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UNCERTAINTIES IN LCA

Parameter uncertainty in LCA: stochastic sampling under correlation

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Abstract

Purpose At the parameter level, data inaccuracy, data gaps, and the use of unrepresentative data have been recognized as sources of uncertainty in life cycle assessment (LCA). In many LCA uncertainty studies, parameter distributions were created based on the measured variability or on "rules of thumb," but the possible existence of correlation was not explored. The correlation between parameters may alter the sampling space and, thus, yield unrepresentative results. The objective of this article is to describe the effect of correlation between input parameters (and the final product) on the outcome of an uncertainty analysis, carried out for an LCA of an agricultural product.

Methods After a theoretical discussion about the statistical concepts on the creation of multivariate random distributions for a Monte Carlo simulation, a LCA case study for potatoes was performed. LCA followed the International Standards Organization guidelines, and the CML baseline characterization method was applied. The functional unit was 1 t of potatoes, while the inputs were restricted to inorganic fertilizers and pesticides. Differences among the two ways to assess uncertainty (with or without correlation) were analyzed through Monte Carlo methodologies, based on the respective estimated probability density functions. In order to demonstrate the effect of correlation on the final outcome, only global warming potential, acidification, and eutrophication impact categories are presented.

Results and discussion The LCA outcome evidenced the highest environmental impact for N-based fertilizers. Environmental impact of the pesticides to the categories considered was minimum, while its contribution in the characterization phase was lower than 10%. Different degrees of correlation were found between the input factors analyzed and also in relation with yield. Uncertainty analysis results indicated a lower uncertainty level for abiotic depletion and global warming when correlation was taken into account, and the Monte Carlo simulations were based on a multivariate sampling space. The results presented allowed the inclusion of the existence of such correlation within the sampling space for a Monte Carlo simulation. Multivariate sampling spaces can be included in LCA uncertainty analysis but only if sensitivity analysis are done previously in order to identify the input factors with the highest contribution to the output uncertainty.

Conclusions The results of an LCA uncertainty analysis at the parameter level may lead to the wrong conclusions when the input parameters are correlated. Under a Monte Carlo procedure, the sampling space derived from univariate or multivariate normal distributions exert a varying degree of error propagation leading to different responses in the uncertainty analysis.

Keywords Agricultural LCA · Error propagation · Input parameters correlation · Monte Carlo simulation · Multivariate sampling distribution · Uncertainty analysis

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1 Introduction

Uncertainty, defined as the error introduced on the outcome due to variability on measurements, lack of data, and deficient model assumptions, has been a subject of intensive study in life cycle assessment (LCA) during recent years. The value of including uncertainty evaluation as an integral procedure has been recognized. Nowadays, this is a recommended practice (ISO 2006a, b), and is an essential tool in order to improve LCA reliability and usefulness for practitioners (Huijbregts et al. 2001, 2003). In all LCA phases, uncertainty continues to be one of the most critical problems, severely affecting the decision process (Reap et al. 2008). Several classifications for the sources of uncertainty within the LCA context have been proposed (Heijungs and Huijbregts 2004). One of the most addressed sources of uncertainty is the variability on input parameters (Reap et al. 2008; Lloyd and Ries 2007). Statistical approaches aim to explicitly incorporate uncertainty into LCA (Heijungs and Huijbregts 2004). Procedures such as Monte Carlo techniques have been used as preeminent tools in LCA to incorporate uncertainty propagation (see, e.g., Heijungs et al. 2004; Huijbregts et al. 2003; Sonnemann et al. 2003). Monte Carlo simulation requires a joint statistical distribution of all parameters to be included in the analysis. Ideally, this multivariate distribution should be derived from statistical analysis of multiple and replicated measurements (Björklund 2002). Nevertheless, incorporating all uncertainties on input parameters is recognized as an unfeasible task, and selection of relevant input parameters contributing to the uncertainty outcome has been one of the recommended approaches (Ciroth et al. 2005).

Although many LCA studies have dealt with uncertainty at the parameter level, most of them have assumed independence between the amount of materials and energy required to manufacture a product (e.g., Ferret et al. 2004; Sonnemann et al. 2003). The lack of knowledge about the correlation structure between parameters and their distributions have been recognized as one of the uncertainty sources when conducting an LCA study (Huijbregts 1998). From a literature survey on uncertainty approaches in LCA, Lloyd and Ries (2007) found that only 29% of the considered studies discussed the issue of interdependency among parameters. Moreover, this survey determined that only 17% of the studies explicitly accounted for parameters correlation within product systems or between alternate product systems when comparative LCAs were carried out (Lloyd and Ries 2007). However, correlation has been addressed for parameter inputs–outcome relationship or when comparing product systems, controlled by the same parameter set (Huijbregts et al. 2003). Björklund (2002), describing Monte Carlo simulation within the LCA context, states that within the first step of the simulation, probability distributions for the inputs are specified with the assumption of parameter independence. The author also recognizes that this assumption may overestimate output uncertainty and proposes the inclusion of an additional parameter in the simulation, one that two dependent variables have in common. However, in reality, assumption of input parameters independence (i.e., univariate distribution) might not represent LCA uncertainty needs and its corresponding outcome. Multivariate probability distributions arise as an alternative to be included in uncertainty analysis when input parameters are correlated or when correlation of any input parameter and the outcome is present to some extent. For a detailed explanation of multivariate probability distributions, the reader is referred to multivariate statistical books such as Johnson and Wichern (1998) or Everitt and Dunn (1991).

The aim of the present article is to apply multivariate sampling techniques to a Monte Carlo simulation as part of an uncertainty analysis at the parameter level in LCA. We will demonstrate the effect of correlation between input parameters and the final product (i.e., functional unit) by comparing univariate and multivariate distributions. To this purpose, the paper is divided in two major sections. The first section is devoted to explaining the statistical background of multivariate sampling and its differences with the univariate sampling procedure. By making use of an artificial dataset, the correlation between input parameters and its effect on the sampling space will be shown. The second section demonstrates, with a real dataset coming from agriculture, how correlation among input parameters and the final product affects the uncertainty of LCA outcomes.

2 Univariate versus multivariate random sampling

Most of the time, input and output distribution in LCA have been treated as univariate, and different types of probability profiles have been used to describe the statistical distribution of a given parameter (see May and Brennan 2003). This assumption implies that the distribution of any of those parameters contains no information about other parameters. Let's consider two input parameters (i and j) necessary for the manufacturing of a certain product. If i and j are assumed to be independent random variables, the total variance is given by

$$\sigma_{i+j}{}^2 = \sigma_i{}^2 + \sigma_j{}^2 \tag{1}$$

and the generation of normal univariate distributions for an input parameter with mean μ can be done independently, following the formula

$$f(y) = \frac{1}{\sqrt{2\pi}\sqrt{\sigma^2}} \exp^{-(y-\mu)^2/2\sigma^2} \tag{2}$$

However, if both variables are correlated, the total variance is defined as

$$\sigma_{i+j}{}^2 = \sigma_i{}^2 + \sigma_j{}^2 + 2\sigma_{ij} \tag{3}$$

where σ_{ij} is defined as the covariance between inputs i and j. In Eq. 3, the covariance term provides a measure of the strength of the linear relationship between input parameters. So obviously, positive covariances are resulting in an increase in total variance and negative ones in a decrease. In this case, an alternative multivariate normal distribution must be used, and its definition is given by

$$f(y) = \frac{1}{\sqrt{2\pi}^p \left|\sum\right|^{1/2}} \exp^{-(y-\mu)' \sum^{-1} (y-\mu)/2} \tag{4}$$

where y and μ are the corresponding vectors of the variables and their means, p represents the number of variables, Σ represents the variance–covariance matrix ($p \times p$, i.e., 2×2 for the present example), and $|\Sigma|$ indicates the determinant of Σ. The variance–covariance matrix Σ for two correlated variables is then defined by

$$\sum = E\left[(y-\mu)(y-\mu)'\right] = \begin{bmatrix} \sigma_i{}^2 & \sigma_{ij} \\ \sigma_{ij} & \sigma_j{}^2 \end{bmatrix} \tag{5}$$

Sometimes, covariance is a difficult term to interpret because it depends on the units in which the two variables are measured; consequently, it is often standardized by dividing by the product of the standard deviations of the two variables to give a correlation coefficient, ρ_{ij} (Everitt and Dunn 1991), where

$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_i{}^2 \times \sigma_j{}^2}} \tag{6}$$

As an example of these statistical concepts, let's assume that the average requirement of input i to produce one piece of a given product was 125 kg with a standard deviation of 23.5 kg, while for input j, the computed average was 55 kg with a standard deviation of 8.7 kg. By making use of these values, sampling spaces were artificially created for two scenarios, assuming independent normal probability distributions for both variables. So, the first scenario considers the absence of correlation between parameters, while for the second one, a ρ_{ij}=0.85 was assumed, resulting in a bivariate normal distribution. The distributions were sampled with the mvrnorm function in the R-language (R Development Core Team 2008).

The simulations for both sampling spaces (i.e., univariate and bivariate normal distributions) are depicted in Fig. 1. The histogram for each situation shows how normality is preserved for both variables, but the presence of the covariance term alters the shape of the bivariate normal distribution. Thus, the covariance term rotates the main axes of the distribution away from the coordinate axes and elongates the distribution. In practical terms, the latter implies that when correlation between parameters is present and it is not taken into account for the computation of the random sampling vectors, the sampling space becomes larger. Consequently, an undetermined number of simulations will make use of parameter combinations that do not reflect the situation observed in the real world yielding a distorted uncertainty analysis.

The latter can be easily checked by looking at the 95% confidence ellipses included in Fig. 1. Each one represents the 95% probability region of the opposite plotted simulation. In that way, it can be confirmed that omitting the correlation will produce a biased Monte Carlo simulation. For instance, the number of univariate sampling points that fall within the ellipse boundaries of the bivariate distribution (see Fig. 1a) was only 63.7% of the 10,000 simulations realized. In other words, 36.3% of the parameter combinations created out of univariate distributions was located outside the real parameter space.

3 Methods

To demonstrate the effect of correlation between input parameters, including the final product, an LCA was performed for the actual potato production system of the Mantaro Valley (11°46′S, 75°30′W). This valley is located in the central highlands of Peru at an average altitude of 3,250 m above sea level. This production system is roughly characterized as a low-input system where almost no mechanization is present and can be defined as a small-holder family-based activity. From 2006 until 2008, 33 production fields were visited every 2 weeks, and information on input data, as well as on the final output (i.e., yield), was collected based on predefined procedures. Measurements on the field were used to quantify the harvested product and the levels of different input factors, completed with direct interviews with the growers. In this zone, only one production cycle can be grown throughout the year, and agricultural species such as potato, barley, wheat, corn, and faba bean among others are regularly planted by growers.

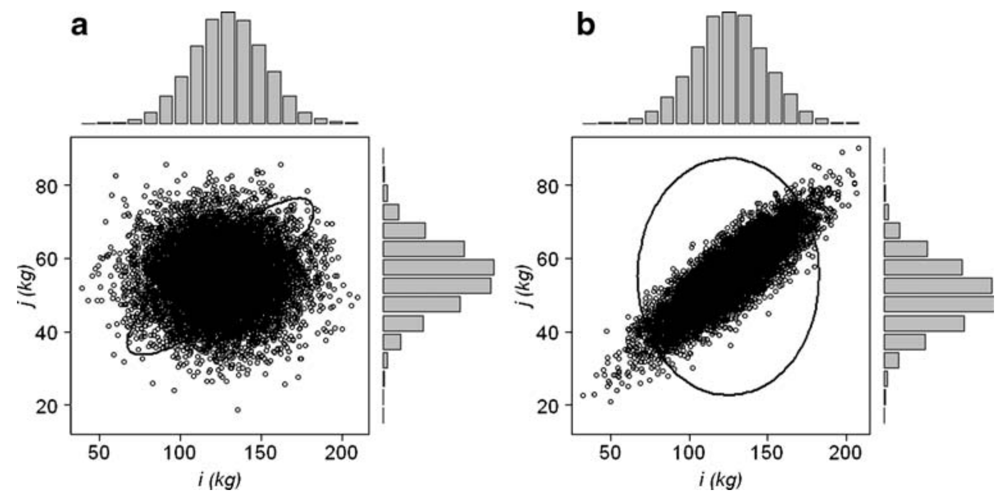

Fig. 1 Comparison of sampling space (n=10,000) for two normally distributed input parameters when (**a**) $\sigma_{ij}=0$, meaning univariate normal distributions for each parameter and when (**b**) $\sigma_{ij}\neq 0$ with $\rho ij=0.85$, which defines a bivariate normal distribution for the sampling space. In each case, the solid line represents the 95% probability region of the opposite distribution, and for each variable, the corresponding histogram was added to depict how normality is preserved under both scenarios

The most common scheme applied in the zone is represented by a 4-year rotation with potato, barley, a leguminous crop (e.g., faba bean), followed by a fallow period.

For the present work, potato cycles were extracted from the general database representing 18% of the total recorded cycles. According to International Standards Organization guidelines (ISO 2006a, b), the goal of this study was to evaluate and compare the environmental performance of the potation production system located in the Mantaro Valley. Additionally, the effect of estimated correlation between input variables and yield on uncertainty propagation is investigated and compared with the case of no correlations. The functional unit was defined as 1 t of potatoes produced during one cropping cycle, and the farm gate was considered as the system boundary. Input factors for the production system were restricted to the most common fertilizers and pesticides applied by growers (see Table 1), since no mechanization is present. For the Life Cycle Inventory phase, background inventory data were based on ecoinvent 2.0 (2007) database, and CML 2 base line 2000 V2.04 characterization method (Guinée et al. 2002) was applied in the Life Cycle Impact Assessment phase. All impact categories proposed by CML were analyzed. However, in the present article, we only present the results for abiotic depletion, eutrophication, and global warming potential with a time horizon of 100 years (GWP100) to demonstrate the effects of correlation on the uncertainty of the LCA outcome.

3.1 Uncertainty analysis

The uncertainty analysis of the correlated input variables was carried out with yield being part of the covariance matrix, because we cannot calculate the uncertainty effect of some correlated input variables without taking into account the existing correlation between these input variables and the final product. In the case of agricultural production, productivity is positively correlated with energy input (Baruah and Dutta 2007), understanding by energy input not only the direct energy used to, e.g., operate vehicles and irrigation pumps but also indirect energy represented by fertilizers, seeds, machinery production, and pesticides (Karkacier et al. 2006). Probability distributions for both univariate and multivariate random sampling were generated, according to the concepts exposed in Section 2 and based on the mean vectors and variance–covariance matrices directly calculated from the data of the potato production system.

Monte Carlo simulation was performed, with 10,000 iterations, for both univariate and multivariate random sampling from normal probability distributions. In order to compare the uncertainty on the LCA outcome under both scenarios, probability density functions (PDFs) were built. The probability of a possible value y_i to lie in some fixed interval $[a, b]$ was calculated by taking the integral of the PDFs of a given impact category following the formula of classical probability theory

$$P(a \leq y_i \leq b) = \int_a^b f(y)dy \tag{7}$$

where $f(y)$ represents the PDF for each impact category. For the present work, only the probabilities of expected values higher than the average μ, i.e., right side of the PDFs, are used to depict the differences on the outcome

of the uncertainty analyses, according to the following formula

$$P(\mu + (\delta \times i) \leq y_i \leq \max(y)) = \int_{\mu+\delta\times i}^{\max(y)} f(y)dy \quad (8)$$

with

$$\delta = \frac{\max(y) - \mu}{100} \quad (9)$$

where i represents the step size subinterval from 0 to 100, while $\max(x)$ indicates the maximum value of the multivariate sample for each impact category. Since we are working with sample distributions, the PDFs have exact limits defined by the range of the Monte Carlo simulations. All statistical analyses were performed with the statistical software R (R Development Core Team 2008).

4 Results

The average amounts, standard deviations, and correlations of the most common agrochemicals used by farmers to grow potatoes in the Mantaro Valley are presented in Table 1. The spectrum of the most used pesticides was reduced to only two active ingredients included in insecticide formulations with a high variability on the dozing, while fertilizers included all macronutrients required by the crop. However, in terms of the general aim of the present work, it is important to emphasize the inherent variability measured on the field. For all input variables considered as well as for the yield, variability observed in the field was high with coefficients of variation ranging from 22% for potassium chloride to 141% in the case of carbofuran. No correlation was determined between metamidophos and urea as well as between metamidophos and potassium chloride. Negative correlation was calculated for both insecticides, while high correlation values were observed between urea and potassium chloride as well as between urea and potato yield. This example depicts the reality of agricultural production where the interactions among agroecological characteristics (e.g., soil properties and climate) and input mass and energy induce a varying response on the final yield not only in space but also in time.

4.1 LCA for the average potato production

Prior to the uncertainty analysis, the LCA for the potato production based on the average measured values is presented next. Table 2 shows the environmental impact caused by each agrochemical on each one of the impact categories defined by CML 2 baseline 2000 V2.04 characterization method. For all impact categories, N-based fertilizers generated the highest environmental burdens with a share higher than 88% in all cases. In the case of eutrophication, diammonium phosphate was responsible for 96.8% of the total impact. The impact of pesticides in all categories was pretty low, being the highest on terrestrial ecotoxicity with a share of 8.1%. Among the pesticides considered, almost the entire impact on each category was attributable to carbofuran.

4.2 Uncertainty analysis

With the correlation matrix presented in Table 1 and with the procedures presented in Section 2, the univariate as well as the multivariate sampling spaces were created in order to compare the differences between both Monte Carlo analyses. A graphical representation of the multivariate sampling space is depicted in Fig. 2. Different linear relationships between the input factors and the final yield are observed when looking at this multivariate sampling space. According to the correlation matrix presented in Table 1, the multivariate sampling space is a more realistic representa-

Table 1 Mean (kg ha^{-1}), standard deviation (SD, kg ha^{-1}), and correlation matrix of the input parameters and the measured yield for an life cycle assessment in potatoes planted in the Mantaro Valley (Peru)

Parameter	Mean	SD	Carbofuran	Metamidophos	DAP	KCl	Urea	Yield
Carbofuran	4.12	5.80	1	−0.75	0.99	0.72	0.50	−0.07
Metamidophos	0.60	0.44	−0.75	1	−0.66	−0.09	0.19	0.71
DAP[a]	375.9	125.9	0.99	−0.66	1	0.81	0.61	0.06
KCl[b]	184.7	40.8	0.72	−0.09	0.81	1	0.96	0.64
Urea	275.9	186.9	0.50	0.19	0.61	0.96	1	0.83
Potato yield	13,164	6,321	−0.07	0.71	0.06	0.64	0.83	1

[a] Diammonium phosphate

[b] Potassium chloride

Table 2 Contributions of the most commonly applied pesticides and fertilizers in potato production at the Mantaro Valley (Peru) to the impact categories defined by the CML 2 baseline 2000 V2.04 method in the characterization phase

Category	Unit	Carbofuran	Metamidophos	DAP[a]	KCl[b]	Urea	Total
Abiotic depletion	kg Sb eq	0.053	0.004	0.292	0.061	0.653	1.064
Acidification	kg SO_2 eq	0.029	0.002	1.266	0.026	0.266	1.589
Eutrophication	kg PO_4 eq	0.001	1.3E-04	1.531	0.004	0.044	1.581
Global warming potential (GWP100)	kg CO_2 eq	4.392	0.352	45.99	7.449	70.601	128.8
Ozone layer depletion (ODP)	kg CFC-11 eq	7.98E-07	5.06E-08	3.88E-06	9.12E-07	9.41E-06	1.51E-05
Human toxicity	kg 1,4-DB eq	2.326	0.160	30.04	5.843	36.263	74.6
Fresh water aquatic ecotoxicity	kg 1,4-DB eq	0.344	0.031	7.082	1.040	4.724	13.2
Marine aquatic ecotoxicity	kg 1,4-DB eq	1,604.7	106.7	19,767.1	1,334.8	15,233.6	38,046.9
Terrestrial ecotoxicity	kg 1,4-DB eq	0.077	0.006	0.388	0.034	0.521	1.027
Photochemical oxidation	kg C_2H_4	0.001	9.05E-05	0.052	0.002	0.011	0.066

[a] Diammonium phosphate

[b] Potassium chloride

tion of the relationships of the input factors and the yield observed in the field.

The pairs-plot in Fig. 2 allows to discriminate the different degrees of correlation between all the factors. A narrower sampling space between carbofuran and diammonium phosphate, urea, and potassium chloride as well as between urea and yield but to a lesser extent indicates the positive correlation between these factors. The negative correlation between metamidophos and diammonium phosphate is clearly represented by the scatter plot. The sampling spaces for factors such as yield and carbofuran or between diammonium phosphate are similar to those created under the univariate sampling procedure indicating no significant correlation.

The PDFs based on univariate and multivariate sampling spaces for the three analyzed impact categories are presented in Fig. 3. While these PDFs follow the same trend for eutrophication, the differences are noticeable for the PDFs of the other two impact categories. For both impact categories, the multivariate PDF shows a reduced variability in comparison with the univariate PDF. Figure 4 depicts the comparison between probability curves for three impact categories, namely, abiotic depletion, eutrophication, and global warming potential. The figures represent the p value for an expected value to be larger than a value to the right side of the mean impact. So, the probability at the origin of the graph represents the p value of exceeding mean impact. For abiotic depletion as well as for global warming potential, the effect of considering a multivariate sampling space is clear, i.e., uncertainty is reduced in comparison with the univariate sampling space. On the contrary, no noticeable effect was observed for eutrophication as both probability curves followed the same trend.

In order to clarify the interpretation of the uncertainty presented in Fig. 4, some examples are presented next. Let's consider the probability of having an expected value higher than 1.2 kg Sb eq for the abiotic depletion category. According to the univariate Monte Carlo procedure, the probability of such event is 0.2, while if the multivariate sampling space is considered, the expected probability is only 0.08 (see Fig. 4a). In the case of global warming potential, let's suppose we want to find the probability of having a value within the range of 10% higher than the average, i.e., 141.68 kg CO_2 eq and the maximum possible. The Monte Carlo simulation with a univariate sampling space yielded a probability of 0.23, while under the multivariate sampling space, the probability was reduced to 0.13 as shown in Fig. 4c. These two examples clearly demonstrate that estimated impact uncertainty is considerably affected by the correlational structure of input variables and yield. Nevertheless, the assumption of reduced uncertainty for a multivariate sampling space cannot be generalized to all cases, since the effect of correlation on the outcome of an LCA will depend on the structure of the variance–covariance matrix.

5 Discussion

In the past, the incorporation of correlation structure at the parameter level has been merely discussed for uncertainty studies in LCA (see Björklund 2002). In the present work, such correlation was taken into account, and its effect was demonstrated explicitly with an example for potatoes production. By considering the real factor space, following a multivariate normal distribution, and thus taking into

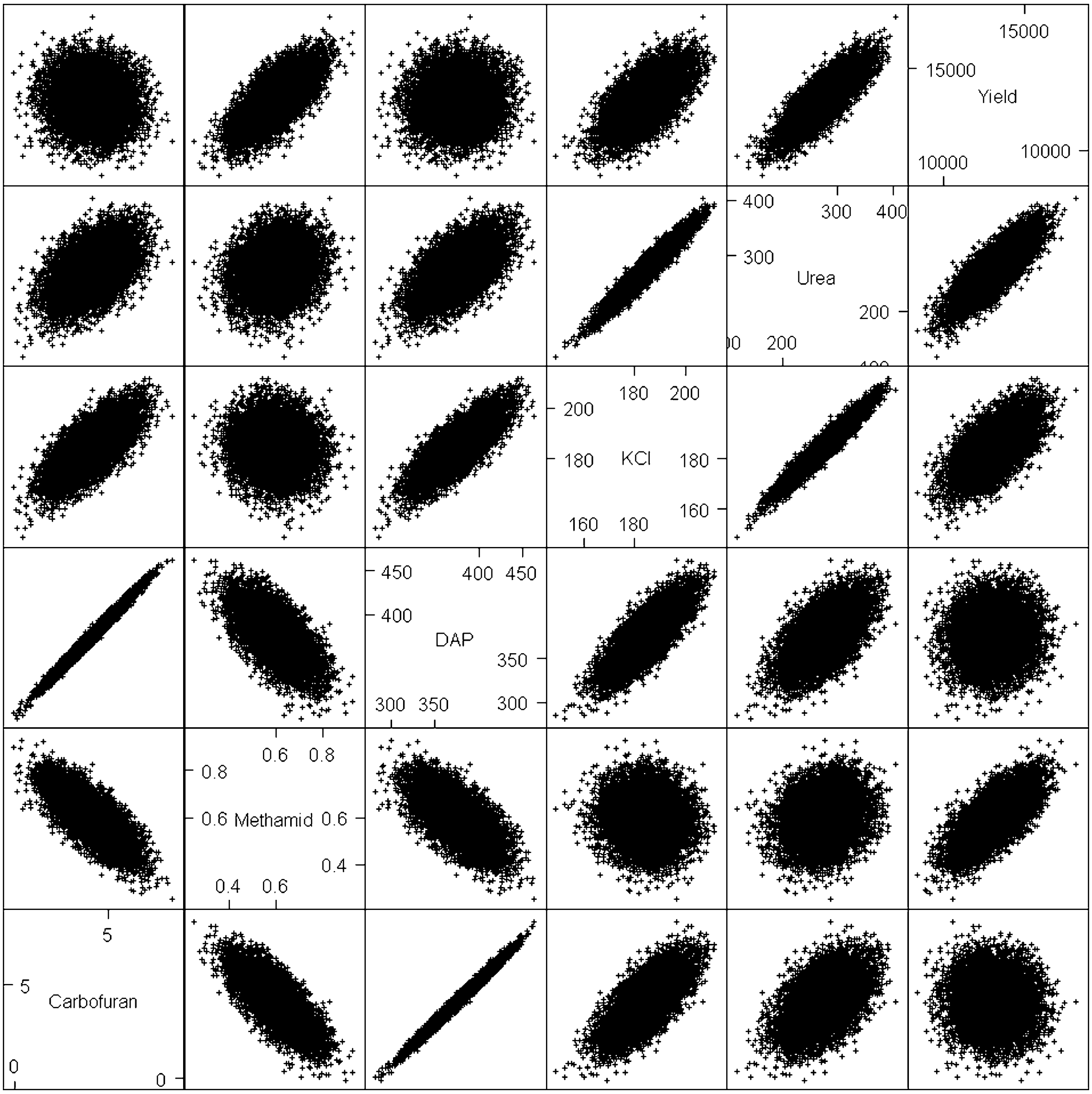

Fig. 2 Scatter plot matrix of the multivariate sampling space created to evaluate the effect of correlation on the outcome of a parameter uncertainty analysis in a life cycle assessment performed for the potato production in the Mantaro Valley (Peru). All input factors and yield are expressed in kg ha^{-1}

account the real correlations between factors, more realistic uncertainty analysis is possible. The described low-input production systems were a typical example of correlation structures occurring between agricultural variables. So, this data were the perfect example to demonstrate the objectives of this article.

Nevertheless, as the manufacture process of a product gains in complexity, it becomes unfeasible to measure enough replicate data for a representative variance–covariance matrix calculation. In that sense, the approach proposed by Huijbregts et al. (2003) can be adapted in order to consider the existence of correlation among input parameters. These authors propose a stratified procedure where prior to the uncertainty analysis, a two-step sensitivity analysis can be performed to identify the parameters that contribute most to the output uncertainty. Once such parameters have been identified, the correlation between such parameters can be analyzed, and the multivariate sampling space can be created for the final Monte Carlo simulations. However, this can only be done if the distributions of the parameters are known and derived from data measured in the field.

6 Conclusions

The effect of correlation between parameters on the impact uncertainty of an LCA was demonstrated by means of an

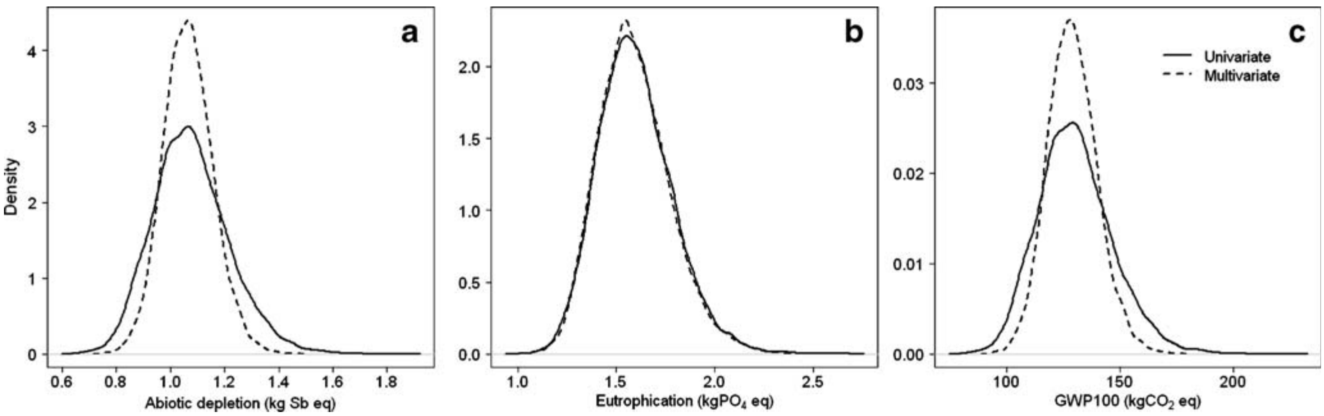

Fig. 3 Probability density functions based on univariate or multivariate sampling spaces for the three impact categories selected to evaluate the effect of correlation of the input data on the uncertainty of a life cycle assessment performed for the potato production system of the Mantaro Valley (Peru)

agricultural case study. LCA in agriculture set the adequate framework due to the inherent variability and correlation structure of biological processes involved in crop production. The choice of a univariate sampling space instead of a multivariate one introduces another source of error whenever data is available to devise distributions and variance–covariance matrixes.

Uncertainty analysis at the parameter level in an LCA, without proper knowledge about the correlation structure among factors, will lead to unrealistic sampling spaces, which in turn, will mislead the results of the analysis. Although in many cases the inventory for a certain product or service may become larger, at least the correlation structure of the most important input factors has to be characterized and used for accurate uncertainty analysis.

7 Recommendations

A properly uncertainty analysis in LCA must consider the correlation among input parameters and also between them and the final product. However, the major drawback to apply this concept in LCA arises from the common impossibility of collecting data from repeated measurements on the field. Alternative strategies such as expert knowledge in order to derive distributions and, on top of that, the correlation dependence structure among factors are not feasible since statistical procedures are mandatory in order to obtain multivariate sampling spaces for a Monte Carlo simulation. Future work may evaluate how significant is the error propagation due to an incorrect sampling space within the overall uncertainty of an LCA.

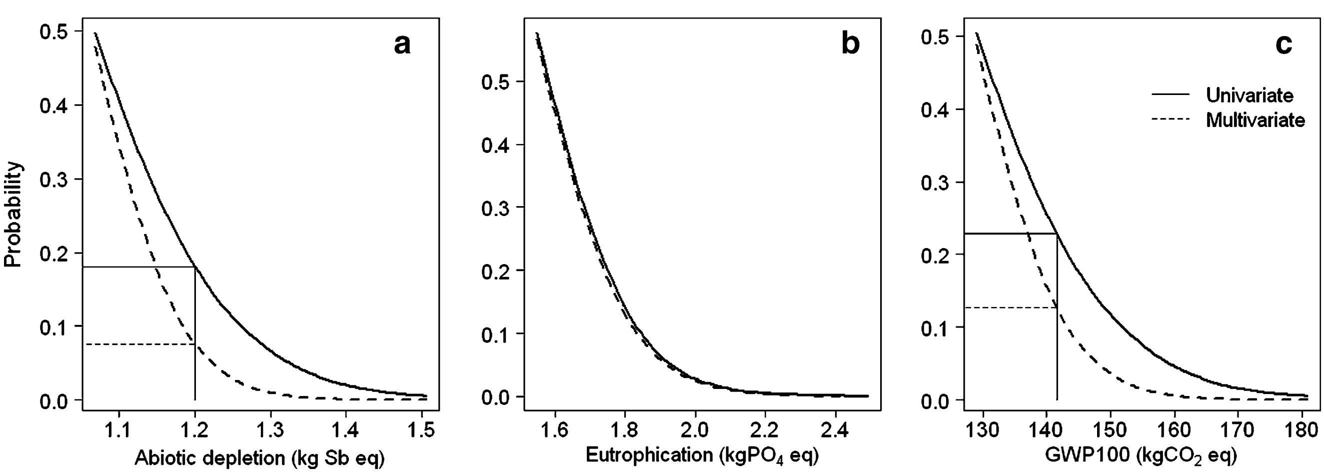

Fig. 4 Expected probabilities of three selected impact categories based on probability density functions considering univariate or multivariate sampling spaces within Monte Carlo simulations to assess the uncertainty at the parameter level on a life cycle assessment for potatoes production in the Mantaro Valley (Peru). Only the probabilities of expected values higher than the average (*right side* of the probability density functions) are presented. *Thinner lines* in (**a**) and (**c**) are used to depict the examples discussed in the text

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